

L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

Structure attributes must be viewed using STN Express query preparation.

=> s l1 ful

FULL SEARCH INITIATED 18:01:46 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 1419 TO ITERATE

100.0% PROCESSED 1419 ITERATIONS

6 ANSWERS

SEARCH TIME: 00.00.01

L2 6 SEA SSS FUL L1

=> d 1-6

L2 ANSWER 1 OF 6 REGISTRY COPYRIGHT 2007 ACS on STN

RN 685564-38-9 REGISTRY

ED Entered STN: 25 May 2004

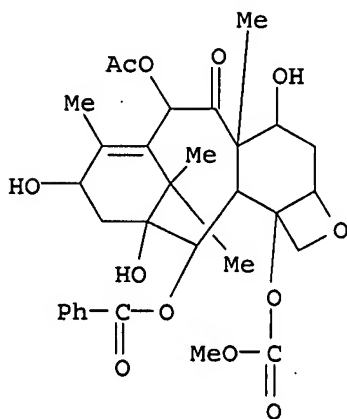
CN Carbonic acid, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-6-(acetyloxy)-12-(benzoyloxy)-3,4,4a,5,6,9,10,11,12,12a-decahydro-4,9,11,?,?-pentahydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-12b(2aH)-yl methyl ester (9CI) (CA INDEX NAME)

MF C31 H38 O14

CI IDS

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER

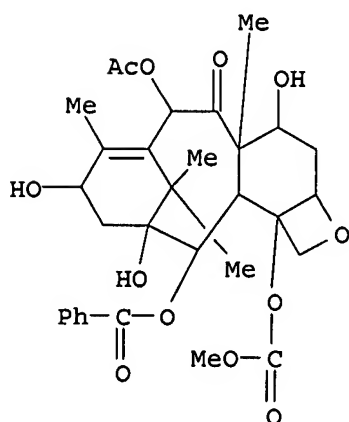


2 ( D1-OH )

1 REFERENCES IN FILE CA (1907 TO DATE)

## 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L2 ANSWER 2 OF 6 REGISTRY COPYRIGHT 2007 ACS on STN  
 RN 685564-30-1 REGISTRY  
 ED Entered STN: 25 May 2004  
 CN Carbonic acid, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-6-(acetyloxy)-12-(benzoyloxy)-3,4,4a,5,6,9,10,11,12,12a-decahydro-4,9,11,?-tetrahydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-12b(2aH)-yl methyl ester (9CI) (CA INDEX NAME)  
 MF C31 H38 O13  
 CI IDS  
 SR CA  
 LC STN Files: CA, CAPLUS, TOXCENTER

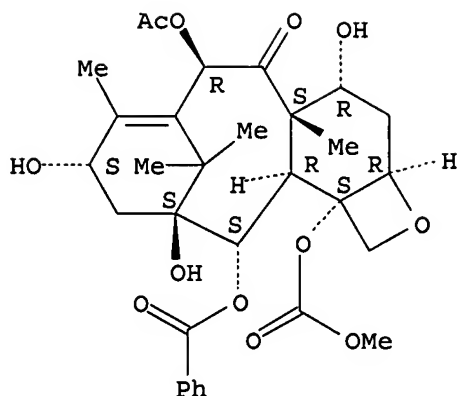


D1-OH

1 REFERENCES IN FILE CA (1907 TO DATE)  
 1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA  
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L2 ANSWER 3 OF 6 REGISTRY COPYRIGHT 2007 ACS on STN  
 RN 685096-39-3 REGISTRY  
 ED Entered STN: 24 May 2004  
 CN Carbonic acid, (2aR,4R,4aS,6R,9S,11S,12S,12aR,12bS)-6-(acetyloxy)-12-(benzoyloxy)-3,4,4a,5,6,9,10,11,12,12a-decahydro-4,9,11-trihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-12b(2aH)-yl methyl ester (9CI) (CA INDEX NAME)  
 FS STEREOSEARCH  
 MF C31 H38 O12  
 SR CA  
 LC STN Files: CA, CAPLUS, TOXCENTER

Absolute stereochemistry.

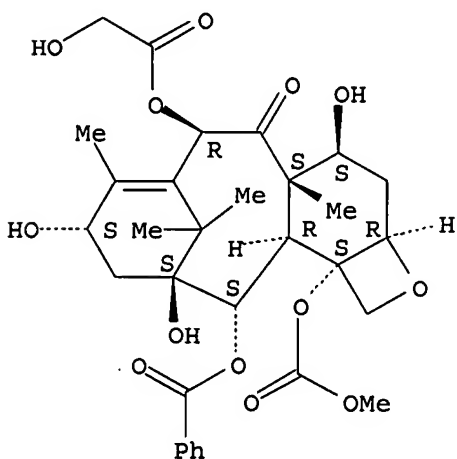


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L2 ANSWER 4 OF 6 REGISTRY COPYRIGHT 2007 ACS on STN  
RN 685096-38-2 REGISTRY  
ED Entered STN: 24 May 2004  
CN Acetic acid, hydroxy-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,9,11-trihydroxy-12b-[(methoxycarbonyl)oxy]-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-6-yl ester (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C31 H38 O13  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER

Absolute stereochemistry.

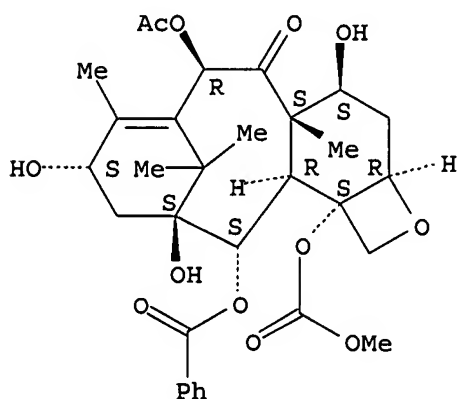


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L2 ANSWER 5 OF 6 REGISTRY COPYRIGHT 2007 ACS on STN  
RN 685096-28-0 REGISTRY  
ED Entered STN: 24 May 2004  
CN Carbonic acid, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-6-(acetyloxy)-12-(benzoyloxy)-3,4,4a,5,6,9,10,11,12,12a-decahydro-4,9,11-trihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-12b(2aH)-yl methyl ester (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C31 H38 O12  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER

Absolute stereochemistry.

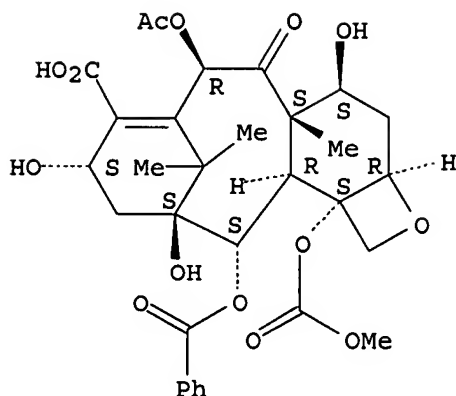


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L2 ANSWER 6 OF 6 REGISTRY COPYRIGHT 2007 ACS on STN  
RN 685096-27-9 REGISTRY  
ED Entered STN: 24 May 2004  
CN 7,11-Methano-1H-cyclodeca[3,4]benz[1,2-b]oxete-8-carboxylic acid, 6-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,9,11-trihydroxy-12b-[(methoxycarbonyl)oxy]-4a,13,13-trimethyl-5-oxo-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C31 H36 O14  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER

Absolute stereochemistry.



1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> fil caplus

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
184.25	212.41

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
0.00	-0.78

CA SUBSCRIBER PRICE

FILE 'CAPLUS' ENTERED AT 18:02:10 ON 07 MAY 2007

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FILE LAST UPDATED: 6 May 2007 (20070506/ED)

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L3 1 L2

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L3 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN

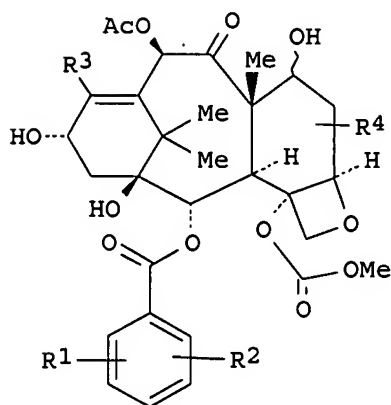
AN 2004:368898 CAPLUS  
 DN 140:375336  
 TI Characterization of taxane metabolites useful as tumor-growth inhibitors  
 IN Comezoglu, S. Nilgun  
 PA Bristol-Myers Squibb Company, USA  
 SO PCT Int. Appl., 113 pp.  
 CODEN: PIXXD2

DT Patent  
 LA English

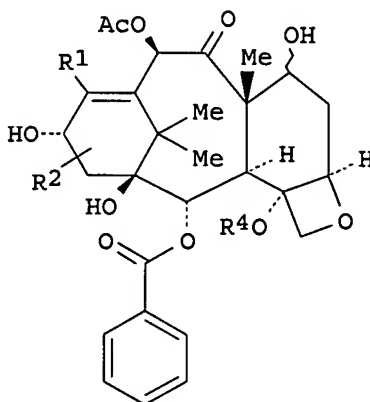
FAN.CNT 1

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PI	WO 2004037211	A2	20040506	WO 2003-US34083	20031024
	WO 2004037211	A3	20040916		
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	RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
	AU 2003285005	A1	20040513	US 2002-421405P	P 20021025
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	EP 1556030	A2	20050727	EP 2003-779320	20031024
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GI



I



II

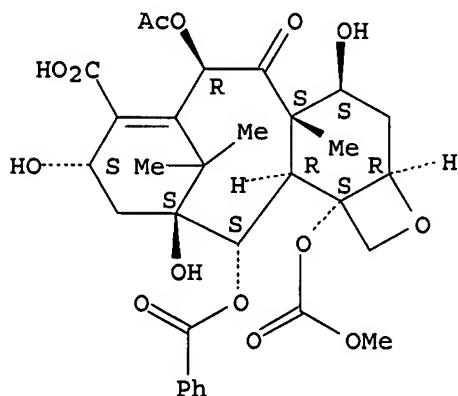
AB This invention relates to compds. that are metabolites of 3'-tert-butyl-3'-N-(tert-butyloxycarbonyl)-4-deacetyl-3'-dephenyl-3'-N-debenzoyl-4-O-(methoxycarbonyl)paclitaxel. The compds., e.g. I [R1 = SG,

OMe, OH, H, ; R2 = H, OH, OMe; R3 = Me, CO2H; R4 = H, OH, (OH)2; SG = SCH2CH(CONHCH2CO2H)NHCOCH2CH2CH(NH2)CO2H] and II [R1 = Me, CO2H; R2 = H, OH; R3 = COMe, H, COCH2OH; R4 = H, CO2Me], or a pharmaceutically acceptable salt, solvate or prodrug, are useful as therapeutic agents, especially as tumor-growth inhibitors. Thus, 14C-, 13C- and unlabeled 3'-tert-butyl-3'-N-(tert-butyloxycarbonyl)-4-deacetyl-3'-dephenyl-3'-N-debenzoyl-4-O-(methoxycarbonyl)paclitaxel were incubated with liver microsomes from various mammals and the metabolites were isolated and characterized.

IT 685096-27-9P 685096-28-0P 685096-38-2P  
685096-39-3P 685564-30-1DP, baccatin-ring hydroxyl regioisomers or epimer  
RL: BMF (Bioindustrial manufacture); BPN (Biosynthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(characterization of taxane metabolites useful as tumor-growth inhibitors)

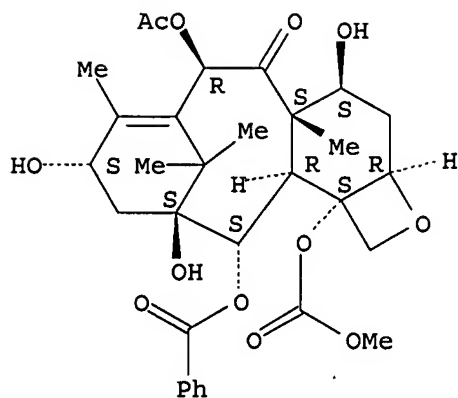
RN 685096-27-9 CAPLUS  
CN 7,11-Methano-1H-cyclodeca[3,4]benz[1,2-b]oxete-8-carboxylic acid, 6-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,9,11-trihydroxy-12b-[(methoxycarbonyl)oxy]-4a,13,13-trimethyl-5-oxo-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 685096-28-0 CAPLUS  
CN Carbonic acid, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-6-(acetyloxy)-12-(benzoyloxy)-3,4,4a,5,6,9,10,11,12,12a-decahydro-4,9,11-trihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-12b(2aH)-yl methyl ester (9CI) (CA INDEX NAME)

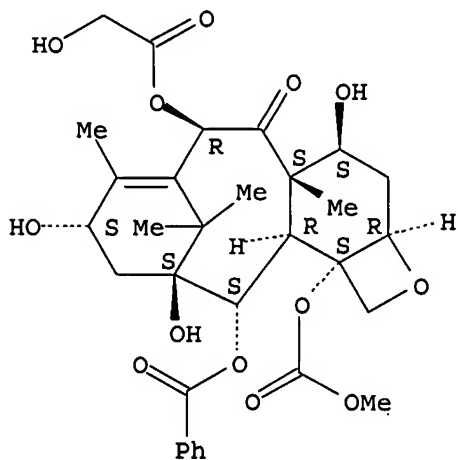
Absolute stereochemistry.



RN 685096-38-2 CAPLUS

CN Acetic acid, hydroxy-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,9,11-trihydroxy-12b-[(methoxycarbonyl)oxy]-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-6-yl ester (9CI) (CA INDEX NAME)

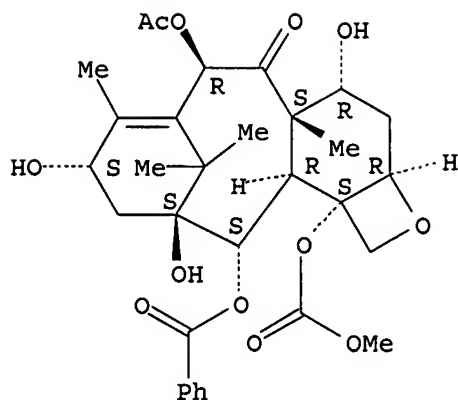
Absolute stereochemistry.



RN 685096-39-3 CAPLUS

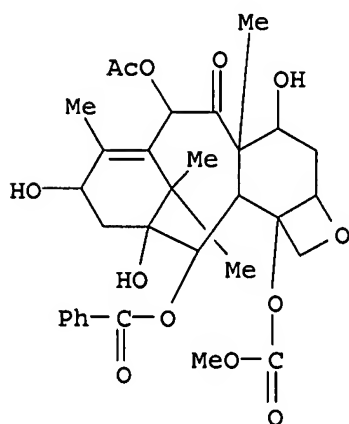
CN Carbonic acid, (2aR,4R,4aS,6R,9S,11S,12S,12aR,12bS)-6-(acetyloxy)-12-(benzoyloxy)-3,4,4a,5,6,9,10,11,12,12a-decahydro-4,9,11-trihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-12b(2aH)-yl methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 685564-30-1 CAPLUS

CN Carbonic acid, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-6-(acetyloxy)-12-(benzoyloxy)-3,4,4a,5,6,9,10,11,12,12a-decahydro-4,9,11,?-tetrahydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-12b(2aH)-yl methyl ester (9CI) (CA INDEX NAME)



D1-OH

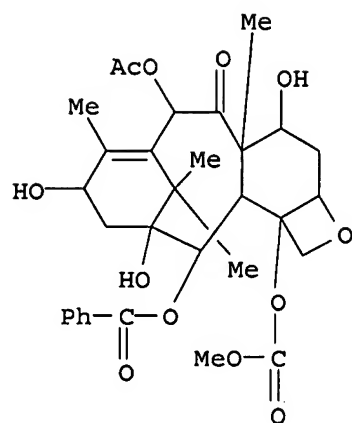
IT 685564-38-9P

RL: BMF (Bioindustrial manufacture); BPN (Biosynthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

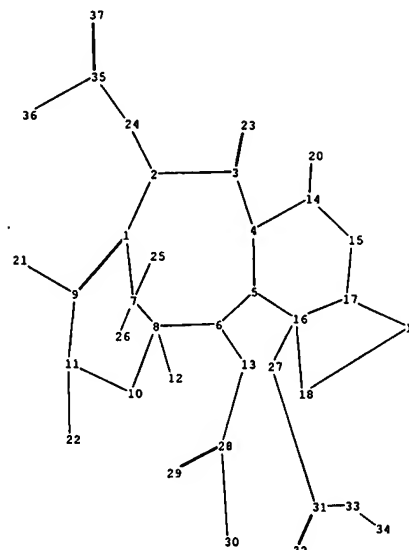
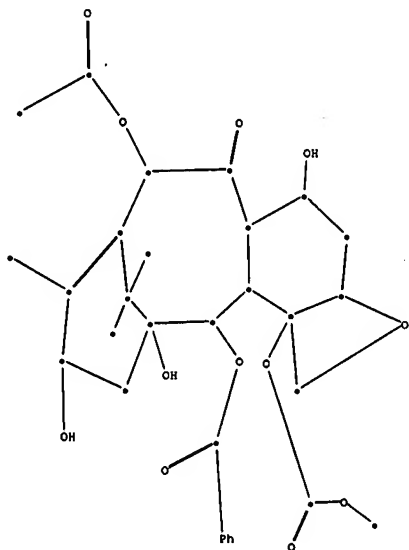
(incubation of, with mammal liver microsomes; characterization of taxane metabolites useful as tumor-growth inhibitors)

RN 685564-38-9 CAPLUS

CN Carbonic acid, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-6-(acetyloxy)-12-(benzoyloxy)-3,4,4a,5,6,9,10,11,12,12a-decahydro-4,9,11,?,?-pentahydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-12b(2aH)-yl methyl ester (9CI) (CA INDEX NAME)



2 ( D1-OH )



chain nodes :

12 13 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 14 15 16 17 18 19

chain bonds :

2-24 3-23 6-13 7-25 7-26 8-12 9-21 11-22 13-28 14-20 16-27 24-35 27-31 28-29 28-30  
31-32 31-33 33-34 35-36 35-37

ring bonds :

1-2 1-7 1-9 2-3 3-4 4-5 4-14 5-6 5-16 6-8 7-8 8-10 9-11 10-11 14-15 15-17 16-17 16-18  
17-19 18-19

exact/norm bonds :

1-2 1-7 1-9 2-3 2-24 3-4 3-23 4-5 4-14 5-6 5-16 6-8 6-13 7-8 8-10 8-12 9-11 10-11  
11-22 13-28 14-15 14-20 15-17 16-17 16-18 16-27 17-19 18-19 24-35 27-31 28-29 31-32  
31-33 33-34 35-37

exact bonds :

7-25 7-26 9-21 28-30 35-36

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:CLASS  
13:CLASS 14:Atom 15:Atom 16:Atom 17:Atom 18:CLASS 19:Atom 20:CLASS 21:CLASS 22:CLASS  
23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS 31:CLASS 32:CLASS  
33:CLASS 34:CLASS 35:CLASS 36:CLASS 37:CLASS

10/532 533

EAST - [space that works.wsp:1]

Search History

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Ref #	Hits	Search Query	DBs
L1	1133	((549/510) or (514/449)).CCLS.	USPAT
L2	364	I1 and paclitaxel	USPAT
L3	46	I2 and metabolite	USPAT
L4	46	I2 and metabolite	US-PGPUB; USPAT

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☐ Shading  
☐ Lines

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☐ Trash

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Print All... Clear All  
Save Selection... Close  
Save All... Help